

Overcoming the Wall in the Semiclassical Baker's Map

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A major barrier in semiclassical calculations is the sheer number of terms that contribute as time increases; for classically chaotic dynamics, the proliferation is exponential. We have been able to overcome this “exponential wall” for the baker’s map, using an analogy with spin-chain partition functions. The semiclassical sum is contracted so that only of order $N \times T^{3/2}$ operations are needed for an N -state system evolved for T time steps. This is typically less than the computational load for quantum propagation, $T \times N^2$. This method enables us to obtain semiclassical results up to the Heisenberg time, which in our example would have required 10^{90} terms if we were to evaluate the sum exactly. This calculation in turn provides new insight as to the accuracy of the semiclassical approximation at long times. The semiclassical result is often correct; its breakdown is nonuniform.

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In previous work it was shown that semiclassical time correlators (and autocorrelation functions in particular) for chaotic dynamical systems can give accurate answers past the log time, where the semiclassical approximation had been thought to break down [1]. The log time is the time it takes a given cell of size h^D (for D degrees of freedom) to visit essentially all other cells. Theoretical justifications showing why the log time is not always expected to be the end of semiclassical accuracy were given [2]. Essentially, it is not the number of terms in the semiclassical sum that should cause a breakdown, but rather more standard concerns about the validity of the stationary phase approximation for each term, which in turn depends on the areas of enclosed regions in phase space. Often, an *algebraic* breakdown is expected, and, perhaps counterintuitively, strong chaos can *improve* the semiclassical expressions by creating healthy areas (greater than \hbar) in the phase plane.

Just beyond the log time in a semiclassical propagation, another problem emerges: the numerical burden of summing over all the classically independent paths leading from the initial position and returning to it. This “ex-

ponential wall” of proliferating contributing orbits has brought many semiclassical calculations to a halt, well before they were actually breaking down. This was the case for the baker’s map [3] and the stadium [1], both of which are completely chaotic. The wall exists for any strongly chaotic system, since the number of contributing terms in a semiclassical propagator grows exponentially with time. (Similar problems besiege the energy domain trace formula [4], where exponential growth occurs with the action or length of the contributing orbits.) The exponential wall is doubly frustrating because it both limits the utility of semiclassical methods as a tool for calculations and hides from view the answer to an important question: when and how do time-domain semiclassical methods break down?

Since a small change in the classical mechanics does not change the quantum mechanics very much, but can change the long-time classical mechanics drastically, intuition suggests that the details of individual classical returning orbits are not important, especially at longer times. A detailed, explicit semiclassical sum over all returning orbits is thus not really necessary. The information in all the returning trajectories at long times is much larger than the information contained in the eigenstates, again suggesting that some summarizing of the classical mechanics would do little harm to the semiclassical sum.

The work of Dittes, Doron, and Smilansky [5], which approximated the baker’s map transfer operator using a finite Fourier transform, successfully achieved such a summarizing of the classical mechanics in a novel way, and provided the first glimpses of breakdown well past the log time. We return at the end to some of the issues they raised about the accuracy of the long-time semiclassical propagation.

The classical baker’s map is a famous paradigm of chaos and mixing. It was quantized first by Balazs and Voros [6], and has received steady attention since then. Such paradigm systems are one of the great strengths of modern chaos theory, because of the qualitative properties that survive translation into many situations.

The classical baker’s map is an area-preserving, discrete map of the unit square onto itself defined by horizontally expanding and vertically compressing the left half of the square so as to map it onto the bottom half, and similarly taking the right half into the top half. The

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map is hyperbolic with constant exponent $\lambda = \ln(2)$ and is smooth everywhere except for a set of measure zero (the “cutting region” $q = 1/2$). For our purposes, a symbolic representation is most convenient: phase space is the set of infinite sequences of zeroes and ones, with a decimal point inserted (the digit following the decimal point identifies the phase space point as being in the left or right half of the square), and the dynamics is given by shifting the decimal point one place to the right at each time step. This description makes it easy to find periodic and homoclinic orbits. (We note that every string γ of length P is naturally associated with a periodic point of period P , the point with symbolic representation $...\gamma\gamma\gamma.\gamma\gamma\gamma...$. Alternatively, if the wavepacket is centered on periodic point $...aaaa.aaaa...$, it may be useful to think of the string β as standing for a homoclinic excursion, with trajectory $...aaaa\betaaaaa...$.)

A quantization preserving the symmetries of the classical system [7] is obtained by choosing an even integer N ($N = 1/h$) and defining a q -basis of states lying at $q = (n + 1/2)/N$, $n = 0..N - 1$, and a p -basis similarly (this quantization corresponds to imposing doubly antiperiodic boundary conditions on the unit square). Planck’s constant h (a dimensionless number, since we have defined phase space area to be unity) serves here as the grid spacing. The dynamics is most easily described in a mixed representation, with the leftmost $N/2$ q -states mapping (through a discrete Fourier transform) to the bottom $N/2$ p -states, and similarly for the remaining part of the Hilbert space. A relative phase between the two blocks in the propagator matrix is undetermined, and leads to a one-parameter family of quantizations. Ignoring this phase, in configuration space the propagator has the matrix form $B = [F_N^{-1}] \begin{bmatrix} F_{N/2} & 0 \\ 0 & F_{N/2} \end{bmatrix}$, where F_N is the discrete Fourier transform on N sites.

A quantity of interest is the quantum autocorrelation function $A^\Psi(T) = \langle \Psi | B^T | \Psi \rangle$, where Ψ is some wavepacket (e.g., a coherent state). This function, and its semiclassical analogue $A_{SC}^\Psi(T)$, when Fourier transformed, provide information on the quantum and semiclassical spectra and eigenfunctions of the system. Although the statistical properties of the autocorrelation function and its Fourier transform, as well as the divergence between these quantities and their semiclassical approximations for large times (low frequencies), are quite interesting objects of study, in this letter we focus on the actual evaluation of $A_{SC}^\Psi(T)$ for particular values of Ψ and T . In contrast with the quantum autocorrelator, which can be computed in polynomial time (by matrix multiplication), the semiclassical autocorrelator can be computed exactly only in exponential time, because of the exponential proliferation of contributing classical paths for large T . We propose a method of approximating this sum that should also be applicable to other systems in which a symbolic dynamics can be used to classify the classical orbits.

We work in the coherent state representation, and begin with a Gaussian centered at $P_{cent} = (q_{cent}, p_{cent})$ in the unit square, with width σ in the q direction. The 2^T classes of possible trajectories are labelled by strings β of T binary digits. Each class of trajectories corresponds to a unique symbolic history; geometrically, a class corresponds to a stretched (in q) and compressed (in p) piece of the original disc in phase space representing the initial Gaussian. The total overlap at time T can be written as

$$A_{SC}^\Psi(T) = a(T) \sum_{\text{strings } \beta} e^{-f(\beta, P_{cent}, \sigma, T)} e^{ig(\beta, P_{cent}, \sigma, T)}, \quad (1)$$

where $a(T)$ falls off exponentially for large T , compensating for the increase in the number of orbits to be summed over, and f and g are quadratic polynomials in q_{cent} , p_{cent} , and β . One can think of the initial Gaussian as freely spreading along the q -direction and contracting along the p -direction for time T , then being cut into pieces and put back into the unit square according to the map. Each piece is part of the stretched Gaussian; thus the universal prefactor $a(T)$. Each term in the sum (1) corresponds to the overlap of the initial Gaussian with one of the stretched pieces. The pieces have acquired a phase g that is specific to the history of each piece; each piece is attenuated depending on its q -position in the stretched Gaussian and also “misses” the p -center of the original Gaussian by some amount, and thus the corresponding overlap is attenuated by a total factor $\exp(-f)$. Specifically, the exponential suppression of a contribution depends on the location of the periodic point P_β associated with string β , relative to the wavepacket center P_{cent} . In terms of the symbolic dynamics, roughly speaking P_β falls inside the wavepacket if the first $\log_2(N)/2$ bits of β match the binary expansion of q_{cent} and the last $\log_2(N)/2$ bits, taken in reverse order, match the expansion of p_{cent} . (This is true for a circular wavepacket ($\sigma = \sqrt{h}$); for an elliptical wavepacket elongated in the q or p directions, the relative importance of the beginning and end of the string will be different, but the total number of bits which are essentially fixed, i.e. $\log_2(N)$, is unchanged.)

The suppression exponent $f(\beta)$ and phase $g(\beta)$ are both quadratic forms in the coordinates of the point P_β , and hence quadratic in the digits of the finite binary string β . This permits the autocorrelator (1) to be written as a partition function for a finite-length spin chain with an external potential and two-body interactions between the spin-1/2 particles. The role of temperature is played by $1/N$.

The “external potential” (i.e. the piece of $-f + ig$ linear in the digits of β) turns out to be important only for the two ends of the chain, in the large- T (long-chain) approximation. Similarly the two-body interactions in the real part $f(\beta)$ are significant only for bits within $\sim \log_2(N)$ of either edge. Thus, for large T , the vast

majority of bits in the string β enter into the expression (1) only through the two-body contribution to the phase $g(\beta)$. This contribution, however, has the form $\exp(i\pi N \sum_{i>j} (\frac{1}{2})^{i-j} \beta_i \beta_j)$, where β_i ($= 0$ or 1) is the i -th bit of string β . Therefore, the relevant “spin-spin interactions” are local, with scale $\log_2(N)$. We can use this fact to approximate the sum by considering blocks of bits, with length of order $\log_2(N)$. These blocks then have only nearest-neighbor interactions, and the sum can be done just as for an Ising chain. The approximation can be improved in a controlled way by increasing the size of blocks used. The result is that to any arbitrary desired accuracy, the semiclassical autocorrelator can be computed in polynomial time for large T , just as is the case for the quantum autocorrelator.

Ignoring factors of order unity, the expected phase error that results from omitting interactions between bits separated by more than the cutoff of C sites goes as $N(\frac{1}{2})^C T^{1/2}$. (The $T^{1/2}$ factor arises from an incoherent sum over T terms.) Because phase errors from different orbits add incoherently, just as the total phases themselves do, this is also expected to be the fractional size of the error in the sum $A_{SC}^\Psi(T)$. Thus, the number of operations required to evaluate the autocorrelator up to some large time T with error ϵ behaves as $NT^{3/2}/\epsilon$, compared with 2^T operations for evaluating this sum exactly. Typically, one wants to take the calculation out to a time of order the Heisenberg time (the inverse of the typical eigenvalue spacing), which is N for the baker’s map. Thus, the computational load is of order $N^{5/2}/\epsilon$, compared with 2^N for obtaining the full semiclassical result. Thus substantial savings can be achieved for large N (where the semiclassical approximation may be expected to be relevant), with minimal loss in precision. The exact *quantum* propagation of a state vector for the Heisenberg time requires order N^3 operations (N^2 multiplies for each of N time steps), more than the contracted semiclassical sum.

We will present numerical data for a wavepacket centered on the period-2 orbit given by $\alpha = 01$. The wavepacket is centered on $(1/3, 2/3)$, well away from any cuts, so the semiclassical approximation is very good even for moderate values of N . (In any case, the behavior of the baker’s map near the cut is the one aspect of this system which is certainly non-generic.) The value of N used in obtaining the data in Fig. 1 is $N = 226$. (Note that a value equal to 2 times a prime number has been chosen to guarantee “generic” behavior, free from number theoretic anomalies. In particular, values of N equal to a power of 2 should be avoided for the standard baker’s map – such values lead to anomalously large recurrences due to coherent interference effects.) The semiclassical autocorrelator is seen to follow the quantum result very closely until about $T = N/4$, at which time higher order quantum effects become noticeable. Even for T comparable to the Heisenberg time, though, some of the behavior of the autocorrelator function is still seen in the semiclassical calculation. We must note, however, that there is a

definite upper bound to the accuracy of the semiclassical approximation in the time domain coming from the non-unitarity of semiclassical physics [5]. If we had taken the calculation out to several times the Heisenberg time, the exponentially growing eigenstates would begin to dominate the autocorrelator, even for a wavepacket located well away from the caustic in the map.

Looking in the energy domain, we find that some spectral peak locations and heights are reproduced very well, while others are reproduced only poorly and yet others not at all. This is consistent with the results obtained in [5]; our interest however is in understanding the semiclassical behavior of individual states (coherent states or eigenstates, for example), because too much information is lost when concentrating only on the trace of the propagator. In particular, though we do not discuss these issues in this letter, the methods of [5] can easily and, in our opinion fruitfully, be extended to study the properties of eigenstates which are well approximated by the semiclassical physics as well as those which are not. Doing this for the baker’s map and other systems should shed light on the nature of the breakdown of the semiclassical approximation at large times.

Although the present paper deals only with the standard baker’s map, the approach described here should be generalizable to other maps. The extension to generalized baker’s maps, with multiple vertical strips of possibly unequal width, seems to be most straightforward. However, systems for which a symbolic description requires a grammar should also be treatable by these methods. Special care will be necessary in applying our approach to systems in which the Lyapunov exponent is either vanishing or very small in some regions of phase space. For such systems, it will not always be the case that the “interactions” between symbols widely separated in time are small, and such phase space regions will therefore need to be treated separately from the “hard chaotic” regions.

We believe the work we report here may also shed light on the energy-domain Gutzwiller trace formula. The trace formula attempts to give individual eigenvalues in terms of purely classical periodic orbits of all lengths. It is derived by stationary-phase Fourier transform from the semiclassical time-domain Green function that we study here, and stationary phase trace over all coordinates. To understand the notorious convergence difficulties of the Gutzwiller trace formula, one should see how long the semiclassical time-domain Green function remains valid. If it fails to reach the Heisenberg time, then blame for failure of the trace formula to predict individual eigenenergies could be laid at the feet of the diffraction and tunneling which degrade the time-domain semiclassical Green function. Further, the methods we use to contract the proliferating homoclinic orbits may suggest new ways to re-sum the trace formula, a subject which has recently seen much attention in the form of cycle expansions and other tools which effectively (and tantalizingly in the light of the time-domain results given here and

earlier) re-order orbits according to time of arrival [8].

Our results extend the work of Dittes, Doron, and Smilansky. We note that their approach, involving a finite Fourier transform of the transfer operator, is completely different from the spin-chain sum used here. Their conclusions about the breakdown were not very optimistic, but they studied mainly the trace of the propagator, rather than its action on particular states. Dittes *et al.* also studied the quasienergy spectrum and attributed the breakdown of the trace to certain quasienergy eigenvalues which had modulus greater than unity (unitarity necessitates unit modulus of the exact results). They cast doubt on the previously claimed algebraic improvement of accuracy with decreasing \hbar [2], because the bad eigenvalues have a damaging effect on the trace. However, the trace in fact cloaks a nonuniform breakdown in phase space of the type that is presaged in earlier work with the baker's map [3]. There it was noted that nonstationary states initiated near the "cut" in the map suffer diffraction after being cut and degrade much more rapidly than states initiated elsewhere. In the present study, we see evidence that the breakdown is indeed very nonuniform, striking some initial nonstationary states more strongly than others, and affecting some semiclassical eigenstates much more than others.

The present work reinforces the hope that approximate evaluation of semiclassical sums will continue to develop as a tool, making many more semiclassical calculations possible. The approximation given here, which depends on symbolic dynamics and draws on analogies with spin-chain partition functions, can be *faster* than doing the quantum mechanics. This is a rare trait in semiclassical approximations to chaotic systems, and represents something of a watershed for semiclassical long time dynamics. (We note that the Dittes, Doron, and Smilansky method requires a matrix representation larger in dimension than the original quantum problem, thus their method is necessarily somewhat slower than doing a full quantum calculation.) These results may hint at possibilities for further progress in work with periodic orbits and the Gutzwiller trace formula [4].

There are strong indications that other maps and dynamical systems will yield to similar simplifications.

Fig. (1a). Semiclassical vs. quantum autocorrelator for initial circular wavepacket centered on $(1/3, 2/3)$ periodic point (phases not shown).

Fig. (1b). Spectrum obtained by Fourier transforming time data shown above.

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